Mass Transport of Water in Teflon Down to Cryogenic Temperatures; a Transient Numerical Analysis

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Solution Method and Results:

The work shown in this document attempts to quantify the water release of Teflon wire insulation, or any other Teflon body, across a broad temperature range. ANSYS workbench was used to obtain the transient numerical solutions at several wire temperatures. Upon analysis of the results it was discovered we can describe all the numerical solutions with a two part piecewise function. Analytical and numerical results were further analyzed to develop a universal equation for the transient mass transport in any material or thickness.

Universal One Dimensional Mass Flux Equation of surface with any thickness:

$$\mathrm{Mass}_{\mathrm{SurfaceFlux}}(t_{ins}, t) := \begin{cases} \left(\phi_{\mathrm{waterMax}} \cdot \sqrt{\dfrac{D_{12}}{\pi \cdot t}}\right) & \text{if } t \le \dfrac{(t_{ins})^2}{2\pi \cdot D_{12}} \\[2ex] \left(\phi_{\mathrm{waterMax}} \cdot D_{12} \cdot \dfrac{\sqrt[4]{2} \cdot \sqrt{\pi}}{t_{ins}} \cdot e^{-\frac{\sqrt{2\pi} \cdot D_{12}}{t_{ins}^{\,2}} \cdot t}\right) & \text{if } t > \dfrac{(t_{ins})^2}{2\pi \cdot D_{12}} \end{cases}$$

Where:

- "$\mathrm{Mass}_{\mathrm{SurfaceFlux}}$" - is a function of time and thickness and gives the mass flux at the surface
- "t" - is time after placed in dry atmosphere, starting fully saturated in (seconds)
- "D_{12}" is the diffusion coefficient through the body
- "$\varphi_{\mathrm{waterMax}}$" is the saturated concentration of water or other diffusing solute
- "t_{ins}" is the thickness of the material, drying on one side, other side adiabadic

The reason for the piecewise function is as the specimen dries out, the mass flux begins to drop sharply and we must begin to describe the flux by the second part of the equation. This time where the flux shifts from one equation to the other is called the dryout time and was found to be:

$$t_{\mathrm{dryout}} = \frac{(t_{ins})^2}{2\pi \cdot D_{12}}$$

Where:

- "D_{12}" is the diffusion coefficient through the body
- "t_{ins}" is the thickness of the material, drying on one side, other side adiabatic

Applying Universal Equation to Teflon Insulation Across Temperature range:

Here we must make D_{12} a function of temperature, while all other variables are constants and known. Using Arrhenius' law to vary the diffusion coefficient, we then include the temperature dependant diffusion coefficient, being:

$$D_{12}(Temp) = D_o \cdot e^{\frac{-U}{k_b \cdot Temp}}$$

Which then makes our surface mass flux describable by:

$$H2O_{SurfaceFlux}(t_{ins}, Temp, t) := \begin{cases} \left(\phi_{waterMax} \cdot \sqrt{\dfrac{D_o \cdot e^{\frac{-U}{k_b \cdot Temp}}}{\pi \cdot t}} \right) & \text{if } t \le \dfrac{(t_{ins})^2}{2\pi \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (Temp)}}} \\ \left[\phi_{waterMax} \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (Temp)}} \cdot \dfrac{\sqrt[4]{2} \cdot \sqrt{\pi}}{t_{ins}} \cdot e^{-\frac{\sqrt{2\pi} \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (Temp)}}}{t_{ins}^2} \cdot t} \right] & \text{if } t > \dfrac{(t_{ins})^2}{2\pi \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (Temp)}}} \end{cases}$$

Where:

- "$H2O_{SurfaceFlux}$" - is a function of thickness, temperature, and time
- "t" - is time after placed in dry atmosphere, starting fully saturated in (seconds)
- "Temp" - is Teflon temperature in (Kelvin)
- "U" - is the activation energy which is estimated at (0.43eV)
- "k_b"- is the Boltzmann constant ($1.381*10^{-23}$ $m^2*kg/K*s^2$)
- "$\varphi_{waterMax}$" is the saturated concentration of water in Teflon (216 grams/m^3)
- "t_{ins}" is the thickness of the material, drying on one side, other side adiabadic
- "$D_{12}(Temp)$ " is the temperature dependant diffusion coefficient
- "D_o" is estimated at (0.73694 cm^2/sec) for Teflon

Graphical Display of Results:

Figure 1 shows the mass flux of water at several temperatures with respect to time for a 400 micron thick piece of Teflon. These temperatures were chosen as they result in mass diffusion coefficients two orders of magnitude lower than the previous. Figure 2 shows the surface mass flux of water at several times with respect to temperature for the same 400 micron thick piece; the times start at 10^2 seconds and increase by one order of magnitude. Figure 3 shows the transient affect of doubling the Teflon thickness several times, keeping temperature constant; results shown for two temperatures. Additional calculations, variables for preparing the numerical model, and other details are contained in Appendix A.

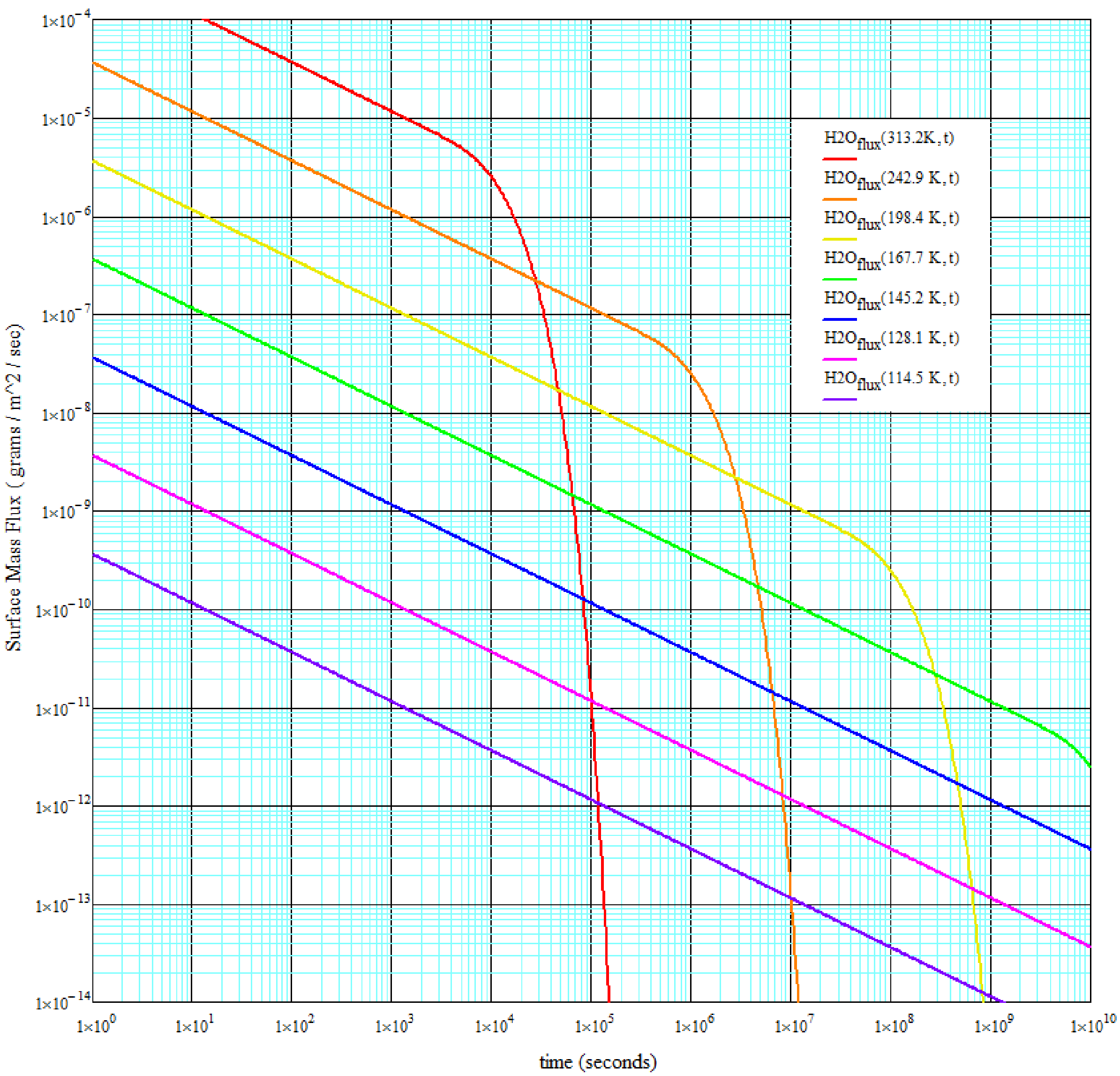


Figure 1: Mass flux of water at several temperatures with respect to time. (400 micron thick specimen)

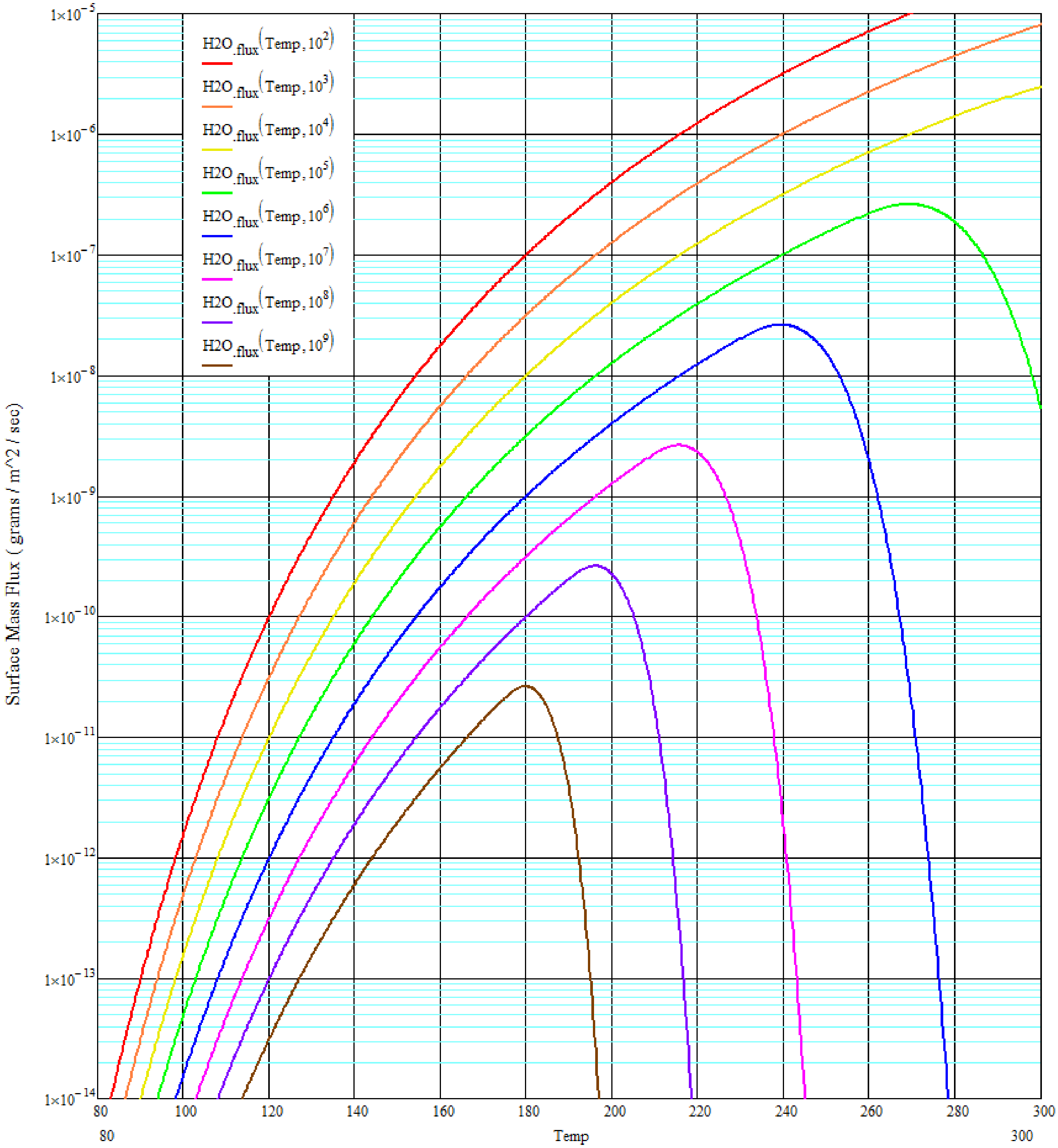


Figure 2: Mass flux of water at several times with respect to temperature. (400 micron thick specimen)

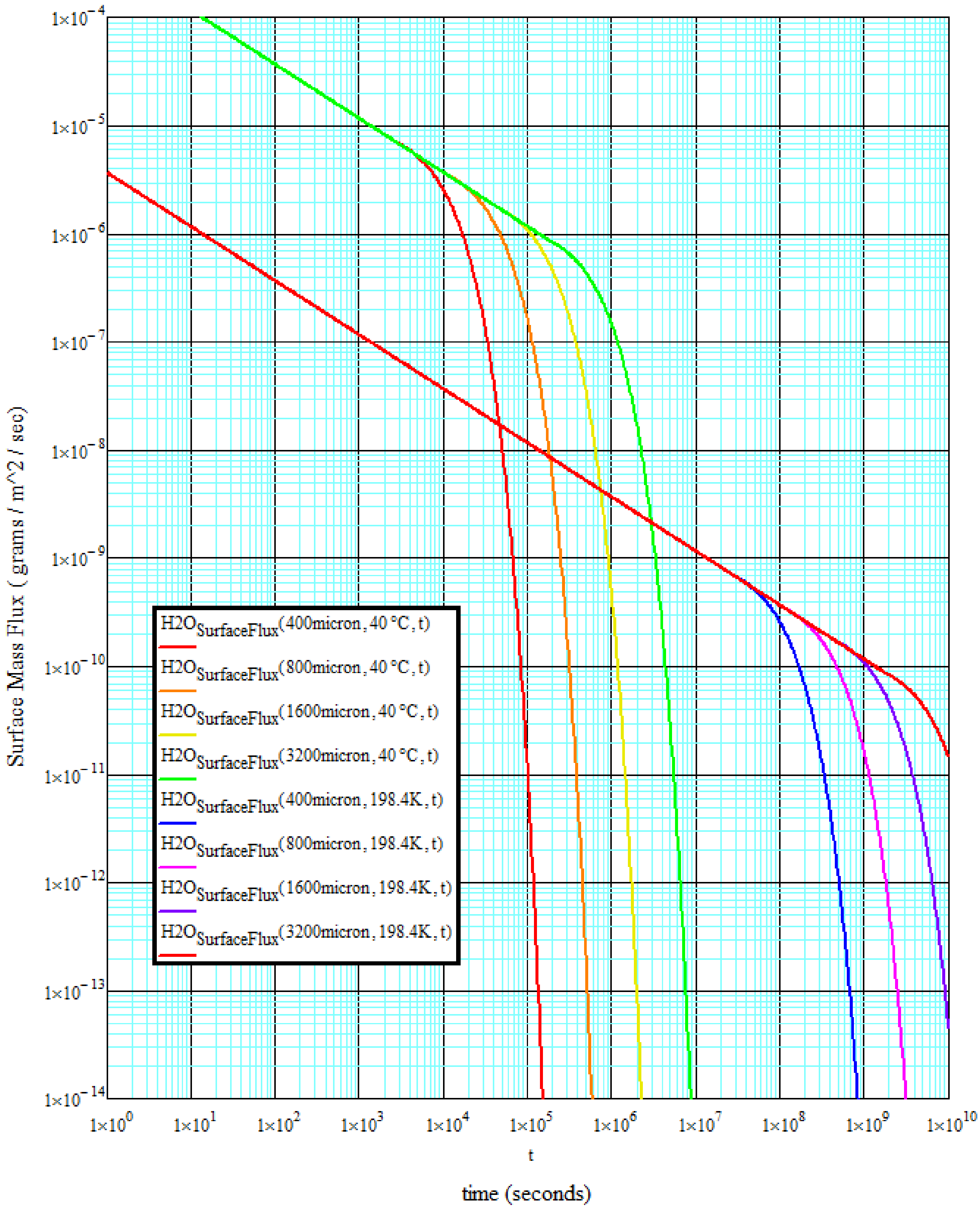


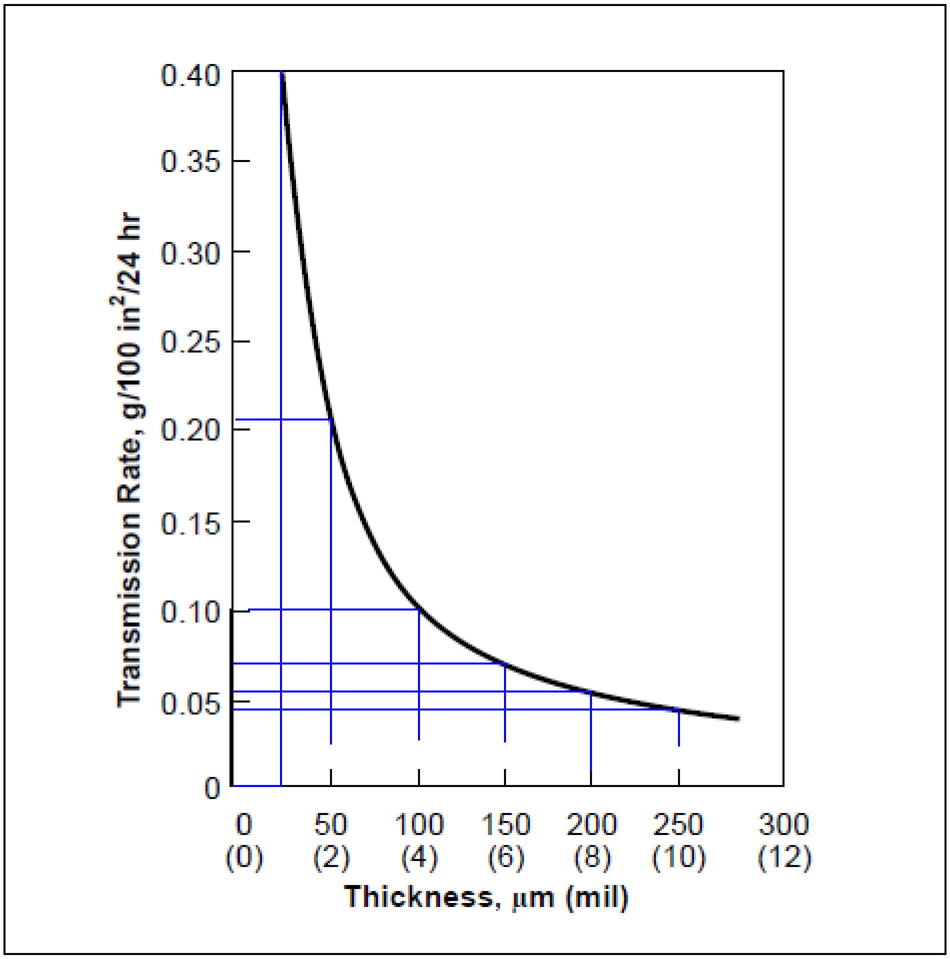
Figure 3: Transient mass flux at two temperatures with four material thicknesses, dryout time quadruples with doubling in thickness.

APPENDIX A

Calculations, Setup, and Results of Numerical Analysis

Measurements of water permeation through Teflon at 40ºC per ASTM E96

http://www.rjchase.com/permeation_effects.pdf



Source: DuPont

This is an almost perfect linear correlation of a constant over the thickness, being:

$$C_{per} := 0.419665$$

$$\mathrm{Flux}(\mathrm{thickness}) := \frac{C_{per}}{\frac{\mathrm{thickness}}{\mathrm{mil}}} \cdot \frac{\mathrm{gr}}{100\mathrm{in}^2 \cdot 24\mathrm{hr}} \qquad \mathrm{Flux}(400\mathrm{micron}) = 0.027 \cdot \frac{\mathrm{gr}}{100\mathrm{in}^2 \cdot 24\mathrm{hr}}$$

$$\mathrm{Flux}(400\mathrm{micron}) = 4.781 \times 10^{-6} \frac{\mathrm{gr}}{\mathrm{m}^2 \mathrm{s}}$$

Properties of Teflon saturated with water (data from outgassing.nasa.gov)

$Solubility := 0.01\%$ $\rho_{Teflon} := 2.16 \frac{gr}{cm^3} = 2.16 \times 10^6 \frac{gm}{m^3}$

$\phi_{waterMax} := Solubility \cdot \rho_{Teflon} = 216 \frac{gm}{m^3}$

$t_{test} := 400micron$

Solving the transport equation

$J = D_{12} \cdot \left(\frac{d}{dx} \phi \right)$ $Rate(t_{test}) = D_{12} \cdot \left(\frac{d}{dx} \phi \right)$

$d\phi_{dx} := \frac{\phi_{waterMax}}{t_{test}}$ $D_{12\_40} := \frac{Flux(t_{test})}{d\phi_{dx}} = 8.853 \times 10^{-12} \frac{m^2}{s}$ *at 40 degrees C*

For estimating diffusion coefficients WRT temperature we use Arrhenius' Law
From Bruce Baller's research(LBNE Doc-3171), Typical Activation energy is 0.43eV $U := 0.43eV$

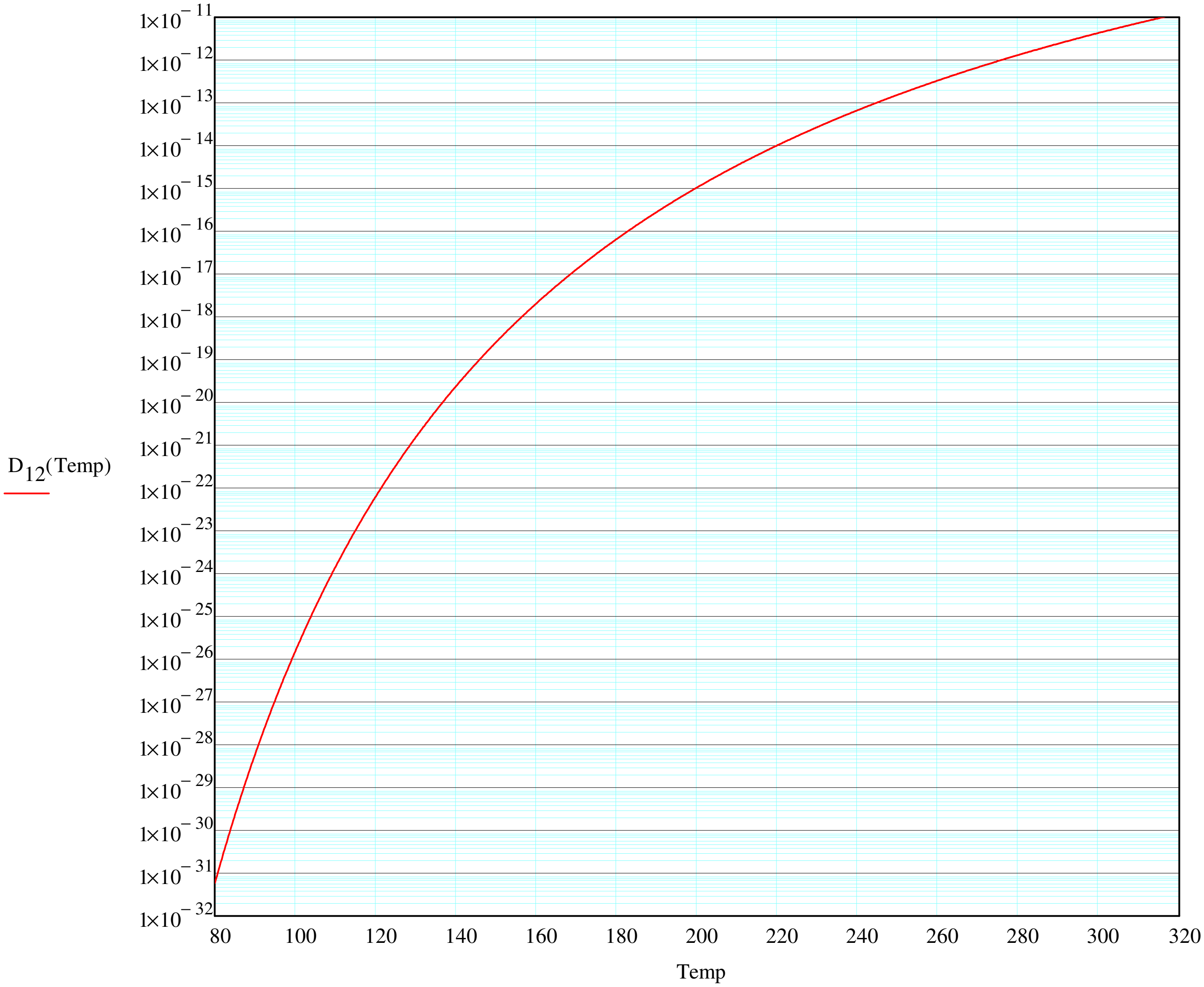
$D_o \cdot e^{\frac{-U}{k_b \cdot 40\,°C}} = D_{12\_40}$

$D_o := Find(D_o) = 7.369 \times 10^{-5} \frac{m^2}{s}$

$D_{12}(Temp) := D_o \cdot e^{\frac{-U}{k_b \cdot Temp}}$

Test that we solved for D_o correctly, (Check for same value)

$D_{12}(40\,°C) = 8.853 \times 10^{-12} \frac{m^2}{s}$ $D_{12\_40} = 8.853 \times 10^{-12} \frac{m^2}{s}$



Since heat and mass transport are analogous to each other we will map the mass to heat energy and solve numerically using an ANSYS Transient Thermal Analysis

Variables for Teflon water transport numerical analysis

$D_{12}(40\,°C) = 8.853 \times 10^{-12}\,\frac{m^2}{s}$ $\qquad \rho_{Teflon} = 2.16 \times 10^{6}\,\frac{gm}{m^3}$ $\qquad \phi_{waterMax} = 216\,\frac{gm}{m^3}$

$$\frac{Cond_{Diff\_Teflon\_40degC} \cdot \phi_{waterMax}}{anythickness} = Flux(anythickness)$$

$$Cond_{Diff\_Teflon\_40degC} := \frac{Flux(400micron) \cdot (400micron)}{\phi_{waterMax}} = 8.853 \times 10^{-12}\,\frac{m^2}{s}$$

Heat to mass mapping

WaterConcentration = Temperature   Mass = Energy   MassFlux = HeatFlux

$$\frac{gr}{m^3} = K \qquad gr = J \qquad \frac{gr}{sec} = \frac{J}{sec} = W$$

$$Cond_{Diff\_Teflon\_40degC} = 8.853 \times 10^{-12} \frac{\frac{gr}{sec}}{m \cdot \frac{gr}{m^3}}$$

Converted to a Thermal Conductance

$$k_{Heat\_Teflon\_40degC} := Cond_{Diff\_Teflon\_40degC} \cdot \left(\frac{\frac{W}{m \cdot K}}{\frac{\frac{gr}{sec}}{m \cdot \frac{gr}{m^3}}} \right) = 8.853 \times 10^{-12} \frac{W}{m \cdot K}$$

Equivalent specific heat for mass transport to temperature mapping

$$c_{pTeflonMass} := \frac{1}{\phi_{waterMax}} = 0.00462963 \cdot \frac{gr}{gr \cdot \frac{gr}{m^3}}$$

Heat to mass mapping

$$\frac{J}{kg \cdot K} = \frac{gr}{kg \cdot \frac{gr}{m^3}}$$

Converted to a Thermal Specific Heat

$$c_{pTeflon} := \frac{1}{\phi_{waterMax}} \left(\frac{\frac{J}{kg \cdot K}}{\frac{gr}{kg \cdot \frac{gr}{m^3}}} \right) = 4.62963 \frac{J}{kg \cdot K}$$

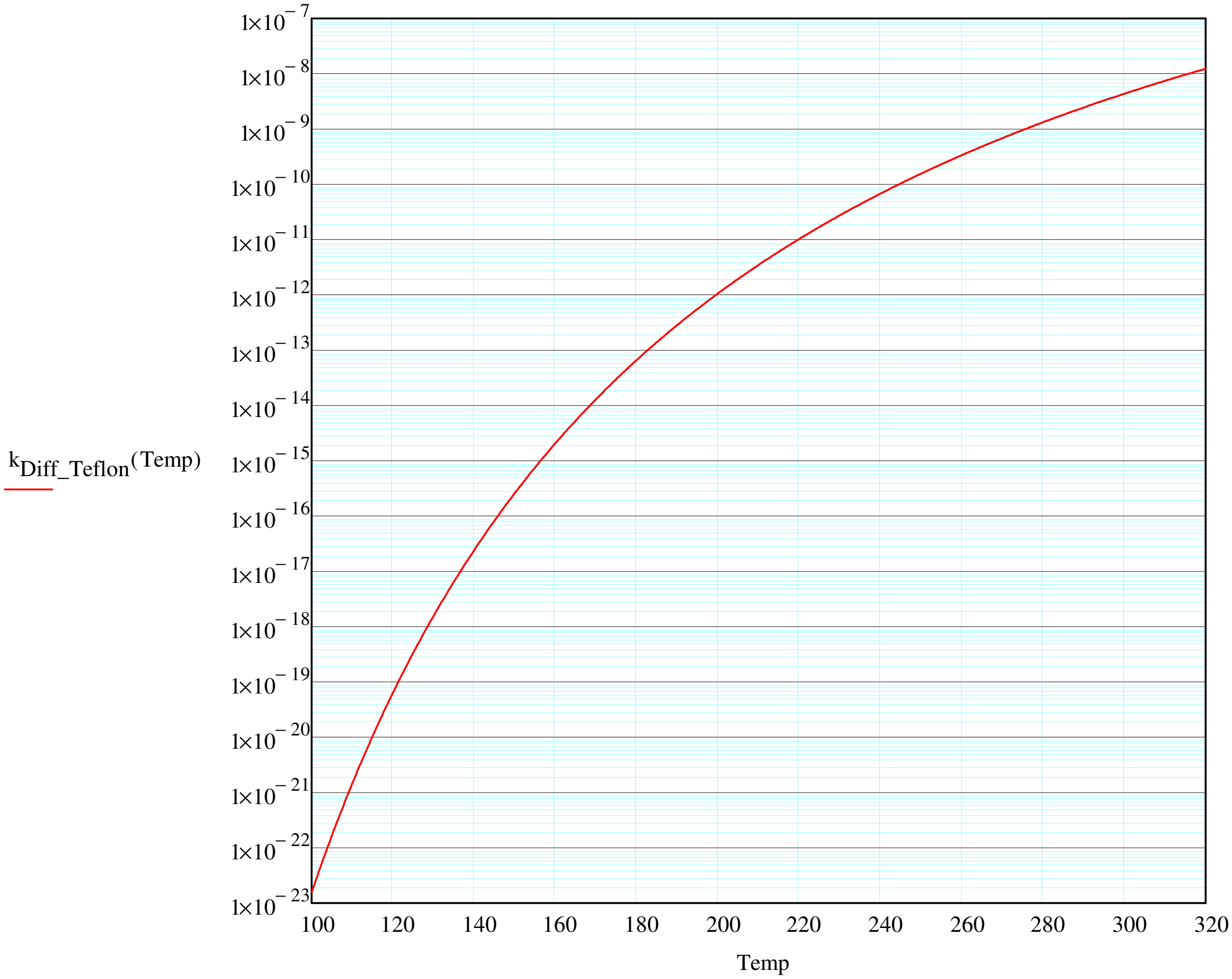
Equivalent Conductivity WRT temperature mass transport to heat energy mapping

$$Cond_{Diff\_Teflon}(Temp) := D_{12}(Temp) \cdot \phi_{waterMax} \cdot c_{pTeflonMass}$$

$$Cond_{Diff\_Teflon}(40\,°C) = 8.853 \times 10^{-12} \frac{m^2}{s}$$

$$k_{Diff\_Teflon}(Temp) := D_{12}(Temp) \cdot \phi_{waterMax} \cdot c_{pTeflon}$$

$$k_{Diff\_Teflon}(40\,°C) = 8.853 \times 10^{-12} \cdot \frac{W}{m \cdot K}$$



Initial and Boundary Conditions and Mapping:

Saturated Teflon at 0.216 kg/m^3 water = 0.216K,

From previous experience (LBNE Doc-3085) we know h.mass and h.heat are can be found by the Lewis number relationship and the Lewis number ~1 for water transport in Argon gas

Typical natural convection and argon properties for reference

$Le := 1 \qquad h_{heat} := 5\,\frac{W}{m^2 \cdot K} \qquad \rho_{Ar} := 3\,\frac{kg}{m^3} \qquad c_{pAr} := 0.52\,\frac{kJ}{kg \cdot K}$

mass convection

$$h_{mass.eq} := \frac{h_{heat}}{\rho_{Ar} \cdot c_{pAr} \cdot Le^{\frac{1}{2}}} = 0.0032 \cdot \frac{\frac{gr}{sec}}{m^2 \cdot \frac{gr}{m^3}}$$

Resistance to mass transport at surface and through Teflon

$$\text{SurfaceFlux} := h_{mass.eq}\cdot\left(\phi_{waterMax} - 0\,\frac{kg}{m^3}\right) = 6.923\times 10^{8}\cdot\frac{nanogr}{m^2\cdot s}$$

$$\text{BodyFlux} := \frac{D_{12}(293K)\cdot\left(\phi_{waterMax} - 0\,\frac{kg}{m^3}\right)}{t_{ins}} = 1597.993\cdot\frac{nanogr}{m^2\cdot sec}$$

$$\frac{\text{SurfaceFlux}}{\text{BodyFlux}} = 4.332\times 10^{5}$$

This shows the bulk motion through the solid Teflon is much more of a resistance than convective diffusion at the surface. Therefore we can initiate the analysis by applying zero concentration at surface as opposed to a convection

Analytical and numerical solutions used to correlate universal piecewise equation for mass transport off the surface of any material. As the thickness increases, as does the dryout time, for an infinitely thick slab, the top equation and analytical solution would be valid throughout all time periods.

Analytical solution for infinite thickness heat equation

$$\text{SurfaceFluxHeat}(t) = \frac{k\cdot\left(T_i - T_{surface}\right)}{\sqrt{\pi\cdot D_{12}\cdot t}}$$

Changing to mass transport equation

$$\text{SurfaceFluxMass}(t) = \frac{\text{Conductance}\cdot\left(\phi_{waterMax} - \phi_{waterSurface}\right)}{\sqrt{\pi\cdot D_{12}\cdot t}}$$

With some simplification we have we then have

$$\text{SurfaceFluxMass}(t) = \frac{\left(\phi_{waterMax} - \phi_{waterSurface}\right)}{\sqrt{\pi\cdot t}}\left(\sqrt{D_{12}}\right)$$

Making this a function of temperature as well, we then get:

$$\text{SurfaceFluxMass}(\text{Temp}, t) = \frac{\left(\phi_{waterMax} - \phi_{waterSurface}\right)}{\sqrt{\pi\cdot t}}\left(\sqrt{D_o\cdot e^{\frac{-U}{k_b\cdot \text{Temp}}}}\right)$$

Universal equation for surface mass flux

$$\text{Mass}_{\text{SurfaceFlux}}(t_{ins}, t) := \begin{cases} \left(\phi_{\text{waterMax}} \cdot \sqrt{\dfrac{D_{12}}{\pi \cdot t}}\right) & \text{if } t \le \dfrac{(t_{ins})^2}{2\pi \cdot D_{12}} \\ \left(\phi_{\text{waterMax}} \cdot D_{12} \cdot \dfrac{\sqrt[4]{2} \cdot \sqrt{\pi}}{t_{ins}} \cdot e^{-\frac{\sqrt{2\pi} \cdot D_{12}}{t_{ins}^{\;2}} \cdot t}\right) & \text{if } t > \dfrac{(t_{ins})^2}{2\pi \cdot D_{12}} \end{cases}$$

Applying Temperature dependence and fixing insulation thickness at 400 micron gives us

$$\text{H2O}_{\text{flux}}(\text{Temp}, t) := \begin{cases} \left(\phi_{\text{waterMax}} \cdot \sqrt{\dfrac{D_o \cdot e^{\frac{-U}{k_b \cdot \text{Temp}}}}{\pi \cdot t}}\right) & \text{if } t \le \dfrac{(t_{ins})^2}{2\pi \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}}} \\ \left[\phi_{\text{waterMax}} \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}} \cdot \dfrac{\sqrt[4]{2} \cdot \sqrt{\pi}}{t_{ins}} \cdot e^{-\frac{\sqrt{2\pi} \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}}}{t_{ins}^{\;2}} \cdot t}\right] & \text{if } t > \dfrac{(t_{ins})^2}{2\pi \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}}} \end{cases}$$

Applying to Teflon and using temperature dependant diffusion coefficient gives us:

$$\text{H2O}_{\text{SurfaceFlux}}(t_{ins}, \text{Temp}, t) := \begin{cases} \left(\phi_{\text{waterMax}} \cdot \sqrt{\dfrac{D_o \cdot e^{\frac{-U}{k_b \cdot \text{Temp}}}}{\pi \cdot t}}\right) & \text{if } t \le \dfrac{(t_{ins})^2}{2\pi \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}}} \\ \left[\phi_{\text{waterMax}} \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}} \cdot \dfrac{\sqrt[4]{2} \cdot \sqrt{\pi}}{t_{ins}} \cdot e^{-\frac{\sqrt{2\pi} \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}}}{t_{ins}^{\;2}} \cdot t}\right] & \text{if } t > \dfrac{(t_{ins})^2}{2\pi \cdot D_o \cdot e^{\frac{-U}{k_b \cdot (\text{Temp})}}} \end{cases}$$